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Dr. Richard S. Miller

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COMPUTED HEATS OF FORMATION OF THREE TETRAAZAPENTALENES, A
TRIS(NITROTRIAZOLO)TRIAZINE, AND A TRICYCLIC *GEM*-
DIFLUORAMINO/TETRANITRAMINE

by

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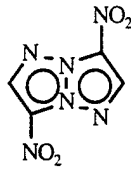
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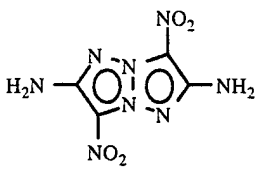
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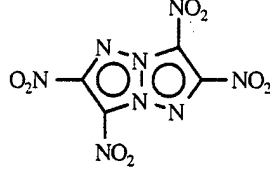
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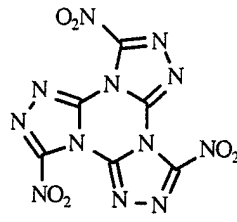
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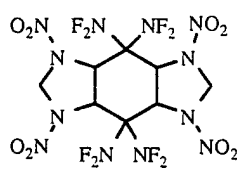
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4



5

1: ΔH_f^{298K} (solid) = 114 kcal/mole = 573 cal/g 4: ΔH_f^{298K} (solid) = 225 kcal/mole = 668 cal/g
2: ΔH_f^{298K} (solid) = 91 kcal/mole = 400 cal/g 5: ΔH_f^{298K} (solid) = 9 kcal/mole = 16 cal/g
3: ΔH_f^{298K} (solid) = 141 kcal/mole = 489 cal/g

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heats of formation; tetraazapentalenes; tris(nitrotriazolo)-triazine; tricyclic gem-difluoramino/tetranitramine

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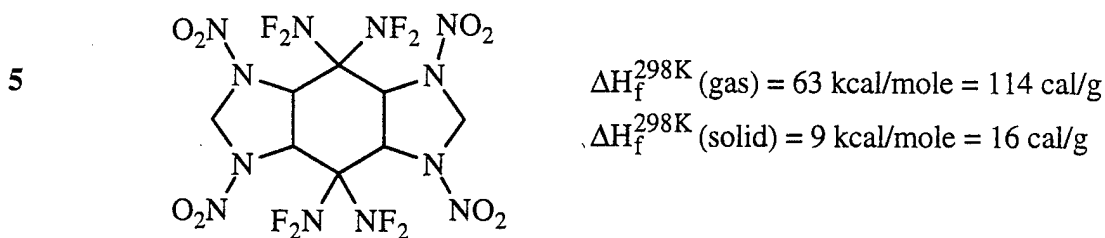
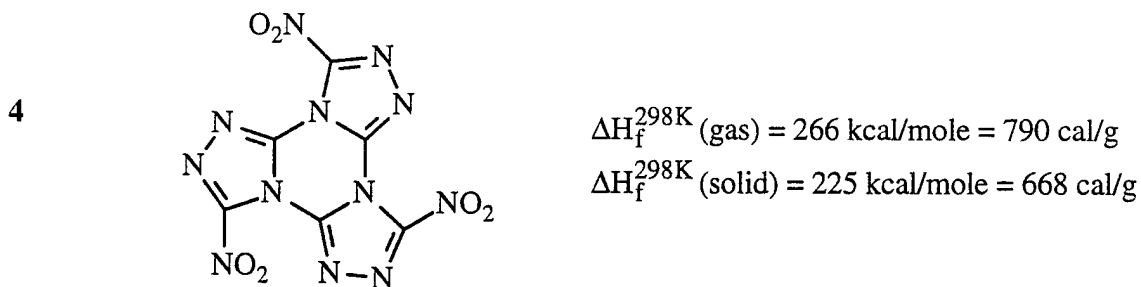
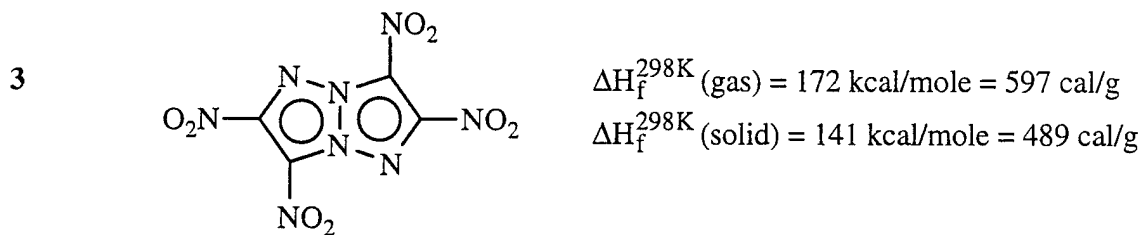
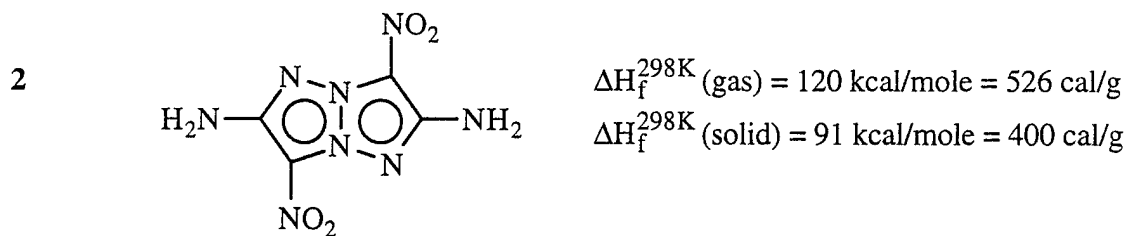
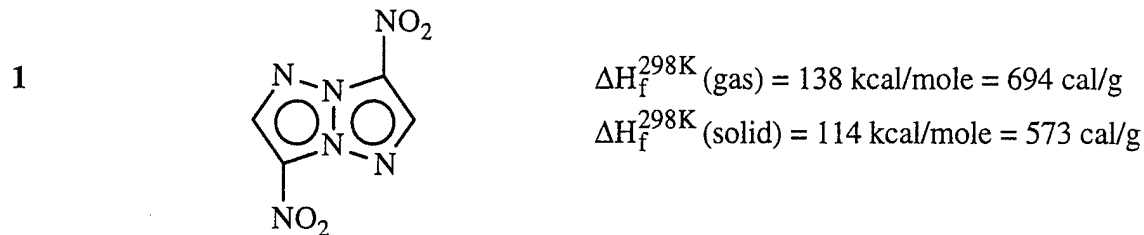
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We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **5**, proposed by W. Koppes and A. Stern (ONR). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat-of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:



For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [4,5].

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